Some integrals related to the Fermi function

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Some elaborations regarding the Hilbert and Fourier transforms of Fermi function are presented. The main result shows that the Hilbert transform of the difference of two Fermi functions has an analytical expression in terms of the Ψ (digamma) function, while its Fourier transform is expressed by mean of elementary functions. Moreover an integral involving the product of the difference of two Fermi functions with its Hilbert transform is evaluated analytically. These findings are of fundamental importance in discussing the transport properties of electronic systems.

I. INTRODUCTION

In many problem in electronic transport calculation the Hilbert transform (HT) of the difference of two Fermi function (FF) is required[1]. Usually this task is accomplished in a numerical way using the Matsubara expansion of FF or other approximate expansions with faster convergence behaviour[2–5]. While these methods as well as the Sommerfeld expansion are of valuable help in numerical work, the importance of exact results can be hardy overlooked.

In this paper I will show that the Hilbert and Fourier transform of the difference of two FF can be expressed in a closed analytical form by means of the digamma function. Moreover an universal integral needed in the theory of electronic transport in presence of phonon scattering[1] is exactly evaluated.

The paper is organized as follow: in Section II a quickly description of the contour integration details used in the work is given; in Section III the main results are derived, while in Section IV an universal integral needed in the discussion of the asymmetric contribution to the current flowing in a molecular wire is worked out. Section V contains the conclusions.

II. HILBERT TRANSFORM

Given a function $g(x)$ its HT is defined as

$$\mathcal{H}(g)(y) \equiv g_H(y) \equiv \frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{g(x)}{y - x} \, \mathrm{d}x \qquad (1)$$

where P is the usual Cauchy principal value.

One powerful technique often used in the evaluation of such kind of integrals extends the function involved in the complex plane and makes use the residua theorem. The typical situation is shown in Fig. 1

By the residua theorem the integral over the closed circuit, done in counter-clockwise way, is proportional to the sum of the internal residua, while the integral over the real axis interval $[A, B] \cup [C, D]$ in the limit of $R \to \infty$, and, separately $r \to 0$ gives the HT desired. More
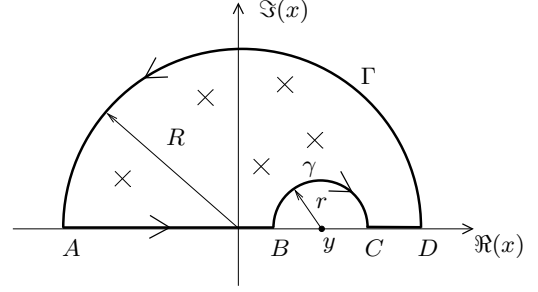

Figure 1: Circuit in the complex plane used to evaluate Hilbert transform. The $\times$ symbols denote the poles of the integrand located at x_n points.

precisely

$$\int_{\text{full circuit}} = 2\pi i \sum_n \text{Res}(x_n)$$
$$= \int_\Gamma + \int_{[A,B] \cup [C,D]} + \int_\gamma \qquad (2)$$

If the integral over the Γ half-circumference vanish in the limit $R \to \infty$ one has

$$2\pi i \sum_n \text{Res}(x_n) = \int_{[-\infty, B] \cup [C, +\infty]} + \int_\gamma, \qquad (3)$$

while in the limit $r \to 0$ the first integral in the right-hand-side of (3) becomes essentially the principal value and the latter can be related to the residuum in y, i.e. $\int_\gamma \to -\pi i \, \text{Res}(y)$, where the minus sign is due to the clockwise orientation of the path.

In summary one arrives at the following result

$$\frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{g(x)}{y - x} \, \mathrm{d}x = 2 i \sum_n \text{Res}(x_n) + i \, \text{Res}(y) \quad (4)$$

where x_n are the poles of $g(x)$ in the $\Im(x) > 0$ half-plane. In case $g(x)$ has no poles on the real axis the preceding formula simplifies as

$$\frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{g(x)}{y - x} \, \mathrm{d}x = 2 i \sum_n \text{Res}(x_n) - i \, g(y). \qquad (5)$$

III. HILBERT AND FOURIER TRANSFORM OF THE DIFFERENCE OF TWO FERMI FUNCTIONS

Let apply the above machinery to the difference of FF

$$g(x) \equiv \frac{1}{e^{\beta_1(x-\mu_1)}+1} - \frac{1}{e^{\beta_2(x-\mu_2)}+1} = f_1(x) - f_2(x) \quad (6)$$

where the chemical potentials μ_i and inverse temperatures β_i can be thought as parameters. The poles structure of g is composed of two infinite series i) $x_n = \mu_1 + (n+1/2)\ 2\pi i/\beta_1$, $n = 0, \pm 1, \pm 2, \dots$ with residua $-1/\beta_1$; ii) $x_m = \mu_2 + (m+1/2)\ 2\pi i/\beta_2$, $m = 0, \pm 1, \pm 2, \dots$ with residua $1/\beta_2$. Only those with $n, m > 0$ are required. Collecting all the contributions one obtains

$$
\begin{aligned}
g_H(y) = +2\,i\ & \sum_{n=0}^{\infty} \left[(x-x_n)\frac{f_1(x)}{y-x} - (x-x_n)\frac{f_2(x)}{y-x} \right]_{x=x_n} \\
+ 2\,i\ & \sum_{m=0}^{\infty} \left[(x-x_m)\frac{f_1(x)}{y-x} - (x-x_m)\frac{f_2(x)}{y-x} \right]_{x=x_m} \\
- i\, & [f_1(y) - f_2(y)] .
\end{aligned}
\quad (7)
$$

Noticing that only the first and the fourth term in the square brackets in the right-hand side are different from zero and equal respectively to $(-1/\beta_1)/(y - x_n)$ and $(-1/\beta_2)/(y - x_m)$, after some straightforward manipulations one obtains

$$
\begin{aligned}
g_H = 2\,i\ \sum_{n=0}^{\infty} \Bigg[& \frac{-1/\beta_1}{y - \mu_1 - (n+1/2)2\pi i/\beta_1} \\
& - \frac{-1/\beta_2}{y - \mu_2 - (n+1/2)2\pi i/\beta_2} \Bigg] \\
- i\,& [f_1(y) - f_2(y)] .
\end{aligned}
\quad (8)
$$

Introducing the quantities $w_j = 1/2 + i\beta_j\,(y - \mu_j)/2\pi$, the sum can be recast in a form that shows the relation with the Euler digamma function Ψ[6,7]

$$\sum_{n=0}^{\infty} \left(\frac{1}{n+w_1} - \frac{1}{n+w_2} \right) = \Psi(w_2) - \Psi(w_1) \quad (9)$$

The term $f_1(y) - f_2(y)$ can be further elaborated exploiting the relation between the Ψ and the FF

$$f(z) = \frac{1}{2} + \frac{1}{\pi}\Im\left[\Psi\left(1/2 - i\,z/2\pi\right)\right] \quad (10)$$

so after some manipulations and remembering that $\Psi(z^*) = \Psi(z)^*$ one finds the analytical result

$$g_H(y;\mu_1,\mu_2,\beta_1,\beta_2) = \frac{1}{\pi}\Re\left[\Psi(w_2) - \Psi(w_1)\right]. \quad (11)$$
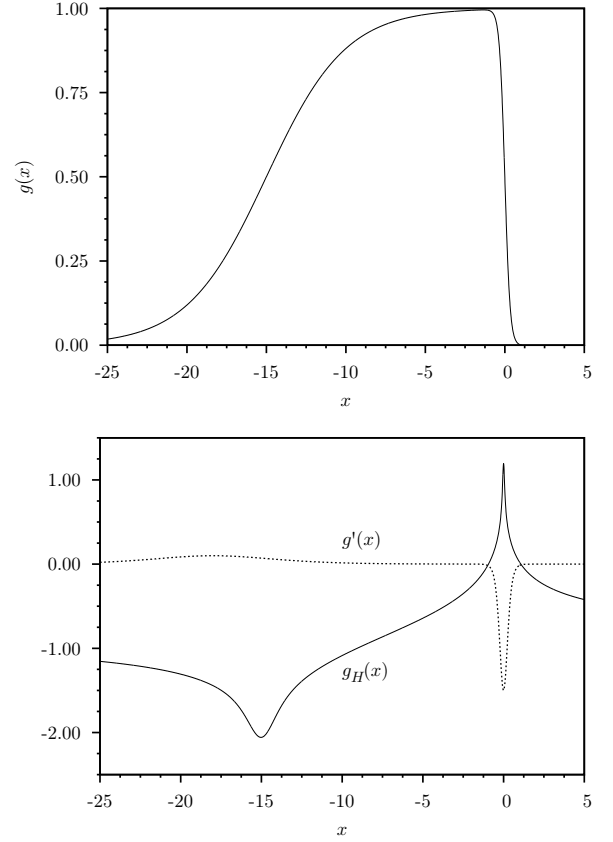
In Fig. 2 a particular case is shown.

Figure 2: (Top) Difference of two Fermi functions. (Bottom) Hilbert transform (solid line) and first derivative (dashed line) of the top panel. The parameters are $\mu_1 = 0$, $\mu_2 = -15$, $\beta_1 = 6$ and $\beta_2 = 0.4$.

Various properties of g_H can be inferred by inspection. For instance

$$g_H(y) = \frac{1}{\pi}\ln\frac{\beta_2}{\beta_1} + \frac{\mu_1 - \mu_2}{y} + O(1/y^2) \qquad |y| \to \infty \quad (12)$$

Moreover if $\beta_1 = \beta_2$, $g(x)$ is even with respect to the point $-(\mu_1 + \mu_2)/2$ while $g_H(y)$ is odd. Finally note that in the low temperature limit $\beta \to \infty$ from the asymptotic expression of the digamma function[6]

$$\Psi(z) = \ln(z) - \frac{1}{2z} + O(z^{-2}) \quad (13)$$

the elementary result

$$g_H(y) = \frac{1}{\pi}\ln\left|\frac{y-\mu_2}{y-\mu_1}\right| + O(\beta^{-2}) \quad (14)$$

is obtained.[8]

The Fourier transform of $g(x)$ can be easily computed with a slight modification of the above procedure. In fact choosing $\lambda > 0$ and using the Jordan lemma closing the

contour in $\Im(x) > 0$ one obtains

$$
\begin{aligned}
g_F(\lambda) &= \int_{-\infty}^{+\infty} \mathrm{d}x \, \mathrm{e}^{i\lambda x} \, g(x) \\
&= \pi i \left[\frac{\beta_2^{-1} \mathrm{e}^{i\lambda\mu_2}}{\sinh(\pi\lambda/\beta_2)} - \frac{\beta_1^{-1} \mathrm{e}^{i\lambda\mu_1}}{\sinh(\pi\lambda/\beta_1)} \right].
\end{aligned}
\tag{15}
$$

The same expression is obtained choosing $\lambda < 0$ and closing the contour in $\Im(x) < 0$. Notice that from this result one can easily evaluate the Fourier transform of g_H by mean of the general relation[8]

$$
\int_{-\infty}^{+\infty} \mathrm{d}x \, \mathrm{e}^{i\lambda x} \, g_H(x) = -i \, \mathrm{sign}(\lambda) \, g_F(\lambda). \tag{16}
$$

IV. EVALUATION OF AN INTEGRAL

Let consider the special case $g_H(x; \omega, -\omega, \beta, \beta)$ and $g(x; 0, -V, \beta, \beta)$, the integral

$$
I = \int_{-\infty}^{+\infty} g(x; 0, -V, \beta, \beta) \, g_H(x; \omega, -\omega, \beta, \beta) \mathrm{d}x, \tag{17}
$$

describes the asymmetrical contribution to the current flowing in a molecular wire[1]. To avoid convergence problems it is better to evaluate the Fourier integral

$$
K(\lambda) = \int_{-\infty}^{+\infty} \mathrm{e}^{i\lambda x} \, g(x; 0, -V, \beta, \beta) \, g_H(x; \omega, -\omega, \beta, \beta) \mathrm{d}x, \tag{18}
$$

from which one obtains $I = K(\lambda \to 0)$. In fact again using the Jordan lemma with $\lambda > 0$ one needs the poles structure of the integrand in $\Im(x) > 0$. Let us define some intermediate quantities to simplify the notation $c_0 = \coth(\pi v_0)$, $c_\pm = \coth(\pi v_\pm)$, $\eta_{\pm\omega} = -(\pm c_0 + c_\mp)/2$ where $v_0 = \beta\omega/2\pi$ and $v_\pm = \beta(V \pm \omega)/2\pi$. Moreover let $z = \exp(-2\pi\lambda/\beta) < 1$. The poles are found straightforwardly:

a) $x_n = \omega + (n+1/2)2\pi i/\beta$, $n = 0, 1, 2, \ldots$ with residua

$$
r_{+\omega}(n) = \frac{i}{\beta} \mathrm{e}^{i\lambda\omega} z^{n+1/2} \eta_{+\omega} \tag{19}
$$

b) $x_n = -\omega + (n+1/2)2\pi i/\beta$, $n = 0, 1, 2, \ldots$ with residua

$$
r_{-\omega}(n) = \frac{-i}{\beta} \mathrm{e}^{-i\lambda\omega} z^{n+1/2} \eta_{-\omega} \tag{20}
$$

c) $x_n = (n+1/2)2\pi i/\beta$, $n = 0, 1, 2, \ldots$, with residua

$$
r_0(n) = \frac{-i}{\pi\beta} z^{n+1/2} \Im\left[\Psi(1 + n + i v_0) + \Psi(-i v_0 - n) \right]; \tag{21}
$$

d) $x_n = V + (n+1/2)2\pi i/\beta$, $n = 0, 1, 2, \ldots$ with residua

$$
\begin{aligned}
r_V(n) = \frac{\mathrm{e}^{i\lambda V}}{2\pi\beta} z^{n+1/2} \times \\
\Big[\Psi(i v_- - n) + \Psi(-i v_- + n + 1) \\
- \Psi(i v_+ - n) - \Psi(-i v_+ + n + 1) \Big].
\end{aligned}
\tag{22}
$$

The integral is thus expressed as

$$
K(\lambda) = 2\pi i \sum_{n=0}^{+\infty} \left[r_{+\omega}(n) + r_{-\omega}(n) + r_0(n) + r_V(n) \right]. \tag{23}
$$

The first two terms are trivial geometric series whose result is

$$
\begin{aligned}
R_\omega &\equiv \sum_{n=0}^{+\infty} \left[r_{+\omega}(n) + r_{-\omega}(n) \right] \\
&= \frac{i}{2\beta} \frac{1}{\sinh(\pi\lambda/\beta)} \left(\eta_{+\omega} \mathrm{e}^{i\lambda\omega} - \eta_{-\omega} \mathrm{e}^{-i\lambda\omega} \right).
\end{aligned}
\tag{24}
$$

For the third term using the results of Appendix A one gets

$$
R_0 \equiv \sum_{n=0}^{+\infty} r_0(n) = \frac{-i z^{1/2}}{\pi\beta} \left\{ \Im\left[S_+(i v_0, z) \right] - \frac{\pi c_0}{1-z} \right\}; \tag{25}
$$

similarly for the last term one finds

$$
\begin{aligned}
R_V &\equiv \sum_{n=0}^{+\infty} r_V(n) = \frac{\mathrm{e}^{i\lambda V} z^{1/2}}{\pi\beta} \times \\
&\left\{ S_+(-i v_-, z) - S_+(-i v_+, z) + i\frac{\pi}{2}\frac{c_- - c_+}{1-z} \right\}.
\end{aligned}
\tag{26}
$$

The integral is now completely solved as

$$
K(\lambda) = 2\pi i \left(R_\omega + R_0 + R_V \right). \tag{27}
$$

To obtain the limiting value $K(0)$ one needs to carefully extract the divergent terms from R_ω, R_0 and R_V

$$
\begin{aligned}
R_\omega &= \frac{i(\eta_{+\omega} - \eta_{-\omega})}{2\pi} \frac{1}{\lambda} \\
&\quad - \frac{\omega}{2\pi}(\eta_{+\omega} + \eta_{-\omega}) + O(\lambda)
\end{aligned}
\tag{28}
$$

$$
\begin{aligned}
R_0 + R_V &= -\frac{i(\eta_{+\omega} - \eta_{-\omega})}{2\pi} \frac{1}{\lambda} \\
&\quad + \frac{i}{\pi\beta} \left[2h(v_0) + h(v_-) - h(v_+) \right] \\
&\quad - \frac{\omega}{4\pi}(c_- + c_+) + O(\lambda),
\end{aligned}
\tag{29}
$$

where the property[6] $\Im(\Psi(i\,x)) = 1/(2\,x) + (\pi/2)\coth(\pi\,x)$ is used and the function $h(x)$ is

$$h(x) \equiv x\Re\big[\Psi(i\,x)\big]. \qquad (30)$$

As expected the divergent terms cancel each other and one gets the final result

$$I = \frac{2}{\beta}\left[h(v_+) - h(v_-) - 2h(v_0)\right]. \qquad (31)$$

Using the asymptotic expansion[6] $h(x) = x\ln(x) + 1/(12x) + 1/(120x^3) + O(x^{-5})$ the limit of low temperature is obtained

$$I = \frac{1}{\pi}\left[(V+\omega)\ln(V+\omega) - (V-\omega)\ln(V-\omega) - 2\omega\ln\omega\right]$$
$$- \frac{2\,\pi\,V^2}{\omega\,(V^2-\omega^2)}\,\beta^{-2} + O(\beta^{-4})$$
$$(32)$$

where the first term is related to the elementary case (14). On the other hand for small x one has[6] $h(x) = \Psi(1) + \zeta(3)\,x^3 + O(x^5)$ ($\zeta(3) \approx 1.202056$) and the limit of high temperature follows

$$I = \frac{12\,\zeta(3)\,\omega\,V^2}{(2\pi)^3}\,\beta^2 + O(\beta^4). \qquad (33)$$

V. CONCLUSIONS

The paper derives analytical results for some integrals related to the difference of two Fermi functions: its Hilbert transform is evaluated in term of the digamma function while the Fourier transform involves only elementary functions. Additionally an exact result useful in the discussion of the asymmetric part of the electronic current in presence of phonon scattering is reported.

Appendix A: A summation formula

The series

$$S_+(w,z) = \sum_{n=0}^{+\infty}\Psi(w+n+1)\,z^n \qquad |z| < 1, \qquad (A1)$$

can be expressed in a closed form[9]. In fact exploiting the telescoping properties of Ψ

$$\Psi(w+n+1) = \sum_{k=0}^{n}\frac{1}{k+w} + \Psi(w) \qquad (A2)$$

and multiplying by z^n and summing one gets

$$S_+(w,z) = \frac{1}{1-z}\,\Psi(w) + \sum_{n=0}^{+\infty}\sum_{k=0}^{n}\frac{z^n}{k+w}. \qquad (A3)$$

The double sum can be decoupled using the rule

$$\sum_{n=0}^{+\infty}\sum_{k=0}^{n}A_{n,k} = \sum_{n=0}^{+\infty}\sum_{k=0}^{+\infty}A_{n+k,k} \qquad (A4)$$

thus obtaining

$$S_+(w,z) = \frac{1}{1-z}\left[\Psi(w) + \phi(z,w)\right] \qquad (A5)$$

where the last term is a particular case of the Lerch transcendent[7] $\phi(z,w) = \Phi(z,1,w)$

$$\Phi(z,s,w) \equiv \sum_{n=0}^{+\infty}\frac{z^n}{(n+w)^s}. \qquad (A6)$$

Notice that ϕ can be also expressed in term of Gauss hypergeometric function[7]

$$\phi(z,w) = \frac{1}{w}\,{}_2F_1(1,w;1+w;z), \qquad (A7)$$

and has a logarithmic singularity in $z = 1$ as can checked from the expansion[6]

$$\phi(z,w) = \sum_{n=0}^{\infty}\frac{(w)_n}{n!}\,(1-z)^n\,\left[\Psi(n+1) - \Psi(w+n) - \ln(1-z)\right] \qquad (A8)$$

which is valid if $|1-z| < 1$ and $|\arg(1-z)| < \pi$.

From the reflection property of the digamma $\Psi(1-z) = \Psi(z) + \pi\cot(\pi\,z)$ follows that $\Psi(w-n) = \Psi(w+n+1) - \pi\cot(\pi\,w)$ and thus

$$\sum_{n=0}^{+\infty}\Psi(w-n)\,z^n = S_+(-w,z) - \frac{\pi\cot(\pi\,w)}{1-z}. \qquad (A9)$$

Moreover

$$\sum_{n=0}^{+\infty}\left[\Psi(-w-n) + \Psi(w+n+1)\right]z^n = 2S_+(w,z) + \pi\frac{\cot(\pi\,w)}{1-z}. \qquad (A10)$$

When $z \to 1^-$ along the real axis, the behavior of $S_+(w,z)$ is easily extracted from (A8)

$$S_+(w,z) = \frac{\Psi(1) - \ln(1-z)}{1-z} + w\left[\Psi(2) - \Psi(w+1)\right]$$
$$- w\ln(1-z) + O(1-z). \qquad (A11)$$

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